Ethylene oxide

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 2.20e-13 cm3/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 5.64e-01

Confidence level: 5.09e-01

Nearest Neighbors from the Training Set

Image not found
Ethylene oxide
Measured: 7.60e-14
Predicted: 2.20e-13

Image not found
1,3-Propylene oxide
Measured: 1.03e-11
Predicted: 6.49e-12

Image not found
Methanol
Measured: 9.44e-13
Predicted: 1.40e-12

Image not found
1,2-Propylene oxide
Measured: 5.20e-13
Predicted: 2.37e-12

Image not found
Dimethyl ether
Measured: 2.98e-12
Predicted: 3.88e-12